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FINAL REPORT

To: OFFICE OF NAVAL RESEARCH (Physics Branch)

Title: COMPUTER SIMULATION OF KINETIC PROPERTIES OF PLASMAS
Contract No. N00014-75-C-0473

Principal Investigator: Jacques Denavit, Professor
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Date: August 1982



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INTRODUCTION

The research was directed toward the development and testing of new numerical methods for particle and hybrid simulation of plasmas, and their application to physical problems of current significance in space physics and in energetic charged-particles systems. This project will terminate on August 31, 1982 and this Final Report describes (I) the research accomplished since the last renewal on April 1, 1981 and (II) a perspective of the work done since the beginning of the project in February 1972.

I. RESEARCH ACCOMPLISHED SINCE LAST RENEWAL

During the present period, research on the project has been concerned with (A) particle diffusion due to stochastic orbits, (B) development of field-implicit hybrid codes; (C) computer studies of ion beams and rings; and (D) saturation of the bump-on-tail instability.

A. Particle diffusion due to orbit stochasticity.

Particle simulation studies of diffusion due to stochastic orbits have been extended to general mode structures with arbitrary electric field amplitudes and phases. This general case requires the computation of particle trajectories by numerical integration methods (e.g. leap-frog), which fail to yield convergent values of the position and velocity of a stochastic particle at a given time. This loss of accuracy, which is the result of rapid amplification of truncation and round-off errors by the K-S entropy, casts some doubts on particle simulations specifically aimed at stochastic effects. To what extent are stochastic effects observed in particle simulations true physics, rather than consequences of computation errors?

This difficulty may be alleviated by using trajectory models, such as the "standard mapping", which do not require numerical integration. However, these models correspond to particular amplitudes and phases and have been found, in our earlier computations, to yield unphysical regularities.

A study of the convergence of stochastic orbit computations was therefore carried out. Since only time or aggregate averages are important in the applications considered, the convergence of numerical integration was tested in terms of these global quantities, rather than in terms of the detailed motions of individual particles. For example, a stochastic orbit tends to fill an entire region of phase space, with the particle visiting every part of

the region if sufficient time is allowed. These regions have complex topologies and boundaries which depend on the amplitudes and phases of the electric field. This study showed that sufficiently accurate numerical integrations can generate such regions with as much accuracy as desired, although the phase points of the particle covering the region always have a large erratic component. This research is presented in the paper "Convergence of Stochastic Orbit Computations," by I. Dilber, J. M. Walsh and J. Denavit, which has been submitted for publication to the Journal of Computational Physics.

B. Development of field-implicit hybrid Monte-Carlo codes.

Recent particle simulation methods with implicit field computation (Mason, J. Comp. Phys. 41, 223 (1981); Denavit, J. Comp. Phys. 42, 337 (1981); Friedman, Langdon and Cohen, Comments Plasma Phys. 6, 225 (1981)) permit the use of large time steps, $\Delta t \gg \omega_{pe}^{-1}$, which are not limited by high-frequency electron oscillations. These methods allow the development of new hybrid codes in which relatively dense and cold plasma components are treated as fluids, while energetic electron or ion are treated as particles.

Computational studies based on hybrid codes of this type could include momentum and energy exchange mechanisms, which are not possible in MHD codes and impractical in particle simulations because of computer limitations. Such codes are expected to play an important role in future computational studies of beam and microwave generation devices.

During the past year, work has proceeded on a one-dimensional electrostatic Hybrid Monte-Carlo (HMC) code designed to address computational issues expected in the development of larger two-dimensional electromagnetic hybrid codes. In this code, ions and thermal electrons are treated as separate

fluids following the equations of Braginskii and including electron inertia. Energetic electrons are treated as particles interacting with the fluids through the field and through collisional energy exchange and Monte-Carlo scattering. Mass exchange between particle and fluid electrons depends on the local density and temperature via the collision frequency, so that the electric fluid can never develop supra-thermal properties inconsistent with a fluid treatment. This experimental code has allowed the study of specific issues related to emission and re-absorption algorithms, particle weights, fluid transport algorithms, zoning and boundary conditions. The results of these studies and examples of applications of HMC will be presented as part of the paper "Time-Implicit Hybrid Simulations and Stochastic Orbit Computations" by J. Denavit and I. Dilber, to be presented at the 24th Annual Meeting of the Division of Plasma Physics of APS, New Orleans, Nov. 1-5, 1982.

C. Computer studies of ion beams and rings.

Research in association with the Laboratory of Plasma Studies at Cornell University has been continued. This work concerns computational studies of azimuthally-symmetric ion beams and field-reversed ion rings with toroidal magnetic fields. Research in this area will be presented in the paper "Hybrid Simulation of Ion Beam Transport in Plasma Cannels" by A. Mankofsky, R. N. Sudan and J. Denavit at the 24th Annual Meeting of the Division of Plasma Physics of APS, New Orleans, Nov. 1-5, 1982.

D. Saturation of the bump-on-tail instability.

Research on the saturation of the single-mode bump-on-tail instability have been completed. The collisionless case and weak collisional effects have been considered. In the collisionless case, a mode close to marginal

stability saturates with a field amplitude $E \approx \Delta^2$, where $\Delta = 2(\omega' - \omega)/\omega' \ll 1$ defines the difference between the mode frequency ω and the frequency ω' of the marginally stable mode. For weak collision frequencies $\nu \sim 10^{-3}\gamma$, where γ is the instability growth rate, much larger saturation amplitudes, $E \approx \Delta^q$, with $q \sim 0.6$ are obtained. These results have been related to analytical theories of the saturation by O'Neil and by Simon and Rosenbluth. This research is presented in the paper "Simulations of the Single-Mode Bump-on-Tail Instability" by J. Denavit, which has been submitted for publication to the Physics of Fluids.

II. PERSPECTIVE OF WORK DONE SINCE BEGINNING OF CONTRACT

This section summarizes and evaluates the activities during the life of the contract, including specifically (A) overall statistics, (B) a scientific perspective, and (C) general observations.

A. Overall statistics.

This contract was initiated on February 2, 1972 and has supported a plasma computational effort at Northwestern University jointly with a contract from the Department of Energy, which was initiated at the same time. Both ONR and DOE contracts will terminate on August 31, 1982.

During this period the ONR contract has supported the equivalent of approximately 18 months of time of the principal investigator, 36 months of research associate (post-doctorate) time, and 48 months of research assistant (graduate student) time.

Two Ph.D. students have done a substantial part of their research on the contract at Northwestern University. In addition, the principal investigator has been closely associated with the research of three Ph.D. students at

Cornell University.

A total of 16 research papers in the Physics of Fluids, the Journal of Computational Physics, Comments in Plasma Physics, and the Journal of Geophysical Research have been published with sponsorship from the contract (see Publications).

B. Scientific perspective.

The general theme of the research under the contract has been on the development of new computer simulation methods and their application to plasmas of interest in space physics and in energetic charged particles systems. These studies, particularly those related to magnetospheric Very-Low-Frequency emissions and to computer simulations of ion beams, were done in close cooperation with the Laboratory of Plasma studies at Cornell University.

The research carried out under the contract since its initiation may be classified according to whether the major contribution was to (1) computer simulation methods or (2) elucidation of new physical phenomena.

1. Computer simulation methods.

- a) Noise in particle simulations, including understanding of how noise is generated (refs. 2, 15), methods to reduce noise (and include collisional effects) by periodic re-initialization using a reconstructed distribution function (ref. 3) and non-random initializations (ref. 16).
- b) Stochastic particles in computer simulations, including the identification of stochastic particles in ion ring particle simulations and of stochastic single-particle instabilities in linearized particle codes (ref. 13), and the study of convergence of

stochastic orbit computations (ref. 18). The occurrence of stochastic single-particle instabilities is an unresolved problem, which remains a major obstacle to further development of linearized particle codes.

- c) The development of particle simulations with large time steps, limited by the condition $\omega_B \Delta t \ll 1$, where ω_B is the bounce (or trapping) frequency, rather than by $\omega_p \Delta t \ll 1$ or $\omega_c \Delta t \ll 1$, where ω_p is the plasma frequency, and ω_c is the electron gyrofrequency. Since $\omega_B \ll \omega_p$, ω_c for most applications these methods considerably extend the domain of application of particle simulations. Two separate concepts were developed: (i) Time steps in which high-frequency oscillations have been integrated and which advance only slowly varying amplitudes and frequencies (ref. 9). This approach has been applied to studies of magnetospheric VLF emissions (refs. 10, 12 and 14) to a study of the saturation levels of the bump-on-tail instability (ref. 17), and by J. L. Vomvoridis and other authors to electron cyclotron oscillation for microwave generation. (ii) Time steps in which high-frequency oscillations are filtered out (ref. 11). This approach has potentially very important applications. It was also developed independently by Mason and is now studied and extended by several other authors.

2. Elucidation of new physical phenomena.

- a) Fundamental studies of the whistler sideband instability (ref. 6) and of the nonlinear elongation of electrostatic and whistler wavepackets due to trapping of resonant particles (ref. 5). In the electrostatic case, this theory of wavepacket propagation has been the object of experimental verification in laboratory plasmas (N. Sato, K. Saeki and R. Hatakeyama, Phys. Rev. Lett. 38, 1480 (1977)).

- b) Numerical and analytical studies of electron heating due to parametric instabilities, including the effect of collisions to suppress the generation of suprathermal electrons (ref. 7).
- c) Comprehensive theoretical studies of magnetospheric Very low Frequency (VLF) emissions, including particle correlations due to interaction with a whistler wave propagating in a non-uniform medium (ref. 10), and the determination of the resulting nonlinear growth rates (ref. 12). A theory of magnetospheric VLF emissions must account for the following features (i) the triggering of monochromatic emissions by signals of sufficient strength and duration, while the background noise and weak short signals are not amplified, and (ii) the occurrence of frequency changes after the emissions have reached sufficiently large amplitude. A nonlinear mechanism exhibiting these features with fixed and varying frequencies was identified and examined analytically and by computer simulation techniques. This mechanism depends on a simultaneous propagation and amplification of wave packets along geomagnetic lines to maintain the nonuniformity ratio $R = VB_0/B_w$ in the regime $|R| \approx 0.5$, corresponding to maximum amplification. (B_0 is the geomagnetic field and B_w is the wave magnetic field). For a constant frequency, this condition yields triggering thresholds related to the properties of the magnetosphere. For a varying frequency $\omega(t)$, it yields the condition $\partial\omega/\partial t \approx \omega_c^2$ for the large-amplitude portion of the risers, where $\omega_c = B_w^{1/2}$ denotes the trapping frequency of the wave (ref. 14).

C. General observations

During the past ten years, computer simulation of plasmas has been a

rapidly growing field of physics and has played an essential role in the development of plasma theory. In addition to this research role, which is expected to continue, computer simulation is also becoming a cost-effective design tool to provide accurate performance predictions for large plasma devices, which are now entering the engineering phase.

Computer simulation of plasmas is generally thought today of comprising two distinct areas:

- (i) Fluid (or MHD) simulation, and
- (ii) Kinetic (including particle, Vlasov and Fokker-Planck) simulation.

Fluid simulation has generally been applied to large-scale problems directly related to the behavior of experimental devices. Kinetic simulation, on the other hand, has generally been applied to basic physical problems in which the particle distributions deviate significantly from a local Maxwellian distribution, such as when wave-particle resonances, trapping or stochastic heating occur. While kinetic simulation usually cannot be directly applied to large-scale problems, their results provide phenomenological models which can be incorporated to some extent into fluid simulations.

Unfortunately, this dichotomy gives a rather imperfect representation of plasmas of interest in space applications or in microwave or beam generation. In most cases these plasmas retain strong non-equilibrium properties, which cannot be incorporated into fluid models, yet occur on long time and space scales, beyond the reach of conventional kinetic simulation. Future progress in computer simulation of plasmas will therefore depend to a significant extent on the development of new hybrid codes, in which dense and relatively cold plasma components are treated as fluids, while energetic components are treated kinetically (e.g. as particles). Such codes are

necessary to treat, for example, interactions between electron or ion beams (or rings) and plasmas, suprathermal components or wall-plasma interaction phenomena. Since a computation can operate only at a single time scale, high-frequency phenomena (such as plasma oscillations) must be eliminated from these hybrid simulations. The recent time-filtering, field-implicit particle simulation methods are therefore an important step in the development of such codes.

Another area of future development in particle simulations concerns linearized particle codes. Most plasma devices (or experiments) are based on two-dimensional equilibria, which are potentially subject to three-dimensional instabilities. It appears difficult in the foreseeable future to perform fully three-dimensional particle simulations on large space-time scales, but linearized particle codes, which compute three-dimensional perturbations of a two-dimensional configuration are practical. Such codes yield at least the initial instability, and in some cases can model saturation resulting from phase mixing of betatron oscillations for example. However, stochastic instability of single particle orbits has been an obstacle to the development of such codes. In essence linearized particle codes follow the separation between two states of a particle (perturbed - unperturbed) and this separation grows exponentially for stochastic orbits, rapidly masking collective phenomena of interest. A method to stabilize such single-particle modes would therefore be an important advance.

In the area of magnetospheric VLF emissions the greatest need appears to be the acquisition of sufficiently reliable data against which the relevance of theoretical models could be tested. Of particular importance would be the simultaneous in situ measurement of the cold electron density, the resonant electron distribution (in the 10-30 keV range), and the pulse amplitude just

before the growth in time occurs. Among theoretical issues of interest in magnetospheric VLF emissions which remain unresolved, is an explanation for the initial generation of variable-frequency waves. Our theory provides a model for amplification of such waves, which allows predictions of their spectral shape in terms of magnetospheric properties. However, the initial generation of such waves appears to require a sideband instability process taking place when an on-frequency emission has reached a sufficiently large amplitude.

PUBLICATIONS

Research carried out since the present Navy contract started has resulted in the following publications:

1. "Theory of Triggered VLF Emissions from the Magnetosphere" by R. N. Sudan and J. Denavit, Physics Today, Vol. 26, No. 12 (Dec. 1973).
2. "Discrete Particle Effects in Whistler Simulation" by J. Denavit, J. Computational Physics, 15, 449 (1974).
3. "Simulation of Collisional Effects in Plasmas" by C. E. Rathmann and J. Denavit, J. Computational Physics, 18, 165 (1975).
4. "Numerical Simulation Methods for Collisional and Turbulent Heating of Plasmas" by C. E. Rathmann, Ph.D. Dissertation, Northwestern University, Evanston, IL 60201 (August 1975).
5. "Effect of Phase-Correlated Electrons on Whistler Wavepacket Propagation" by J. Denavit and R. N. Sudan, Phys. Fluids, 18, 1533 (1975).
6. "Whistler Sideband Instability" by J. Denavit and R. N. Sudan, Phys. Fluids, 18, 575 (1975).
7. "Collisional Effects on Electron Heating Due to Parametric Instability" by J. Denavit, Phys. Fluids, 19, 972 (1976).
8. "Nonuniform Whistler Mode Propagation" by J. L. Vomvoridis, Ph.D. Dissertation, Northwestern University, Evanston, IL 60201 (June 1978).
9. "Long-Time-Scale Simulation of Resonant Particle Effects in Langmuir and Whistler Waves" by C. E. Rathmann, J. L. Vomvoridis and J. Denavit, J. Computational Physics, 26, 408 (1978).
10. "Test Particle Correlation by a Whistler Wave in a Nonuniform Magnetic Field" by J. L. Vomvoridis and J. Denavit, Phys. Fluids, 22, 367 (1979).
11. "Numerical Solutions of the Vlasov Equation with Filtering in Time" by T. L. Crystal, J. Denavit and C. E. Rathmann, Comments on Plasma Physics, 5, 17-28 (1979).
12. "Nonlinear Growth of a Monochromatic Whistler Wave in a Nonuniform Magnetic Field" by J. L. Vomvoridis and J. Denavit, Phys. Fluids, 23, 174 (1980).
13. "A Linearized 3-D Hybrid Code for Stability Studies of Field-Reversed Ion Rings" by A. Friedman, R. N. Sudan and J. Denavit, Journal of Computational Physics, 40, 1 (1981).
14. "Theory and Computer Simulations of Magnetospheric Very-Low-Frequency Emissions" by J. L. Vomvoridis, T. L. Crystal and J. Denavit, Journal of Geophysical Research, 87, 1473 (1982).

15. "Pitfalls in Particle Simulations and in Numerical Solutions of the Vlasov Equation" by J. Denavit, Proceedings of Conference on Mathematical Methods of Plasma Physics (Oberwolfach, Sept. 1979) Methoden and Verfahren der mathematischen Physik, 20, Verlag Peter D. Lang.

The research carried out during the current period (1 April 1980 - 31 August 1982) has resulted in the following publications:

16. "Nonrandom Initializations of Particle Codes" by J. Denavit and J. M. Walsh, Comments on Plasma Physics, 6, 209 (1981).
17. "Simulations of the Single-Mode Bump-on-Tail Instability" by J. Denavit, submitted to The Physics of Fluids.
18. "Convergence of Stochastic Orbit Computations" by I. Dilber, J. M. Walsh and J. Denavit, submitted to the Journal of Computational Physics.

OTHER RESEARCH FUNDS

As stated in the Introduction, this project has been supported jointly by the Office of Naval Research and by the Department of Energy. The present DOE contract terminates on August 31, 1982.

NOTE:

The National Center of Atmospheric Research (NCAR) had supported the research in VLF emissions with grants of CDC 7600 and CRAY-I computing time.

PERSONNEL AND TIME ALLOTMENT

During the present period, research on the project is carried out by the following personnel:

1. Principal Investigator

Professor J. Denavit, 1 September 1981 - 15 September 1981
15 March 1981 - 15 June 1981
16 June 1982 - 30 June 1982

2. Research Associate

Dr. Thomas L. Crystal, 1 April 1981 - 15 July 1981

3. Research Assistants

John M. Walsh, 16 June 1981 - 15 July 1981
Ilhan Dilber, 1 April 1981 - 31 July 1981
1 September 1981 - 15 September 1981
16 December 1981 - 31 July 1982

INSTITUTION PARTICIPATION

During the present period the University has contributed to the project by providing 5% of the academic salary of the principal investigator.

UNEXPENDED FUNDS AT PRESENT TERMINATION DATE

Approximately \$30,000 remained unexpended at the present termination date. These funds were the object of a deobligation (modification A00002 of 16 August 1982).